

Microlocal properties of scattering matrices*

Shu NAKAMURA[†]

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Abstract

We consider scattering theory for a pair of operators H_0 and $H = H_0 + V$ on $L^2(M, m)$, where M is a Riemannian manifold, H_0 is a multiplication operator on M and V is a pseudodifferential operator of order $-\mu$, $\mu > 1$. We show that a time-dependent scattering theory can be constructed, and the scattering matrix is a pseudodifferential operator on each energy surface. Moreover, the principal symbol of the scattering matrix is given by a Born approximation type function. The main motivation of the study comes from applications to discrete Schrödinger operators, but it also applies to various differential operators with constant coefficients and short-range perturbations on Euclidean spaces.

1 Introduction

Let M be a smooth d -dimensional complete Riemannian manifold with a smooth density m , and let $p_0(\xi)$, $\xi \in M$, be a real-valued smooth function on M . We define

$$H_0\varphi(\xi) = p_0(\xi)\varphi(\xi), \quad \varphi \in D(H_0) = \{\varphi \in L^2(M, m) \mid p_0\varphi \in L^2\}$$

be the multiplication operator by p_0 on $\mathcal{H} = L^2(M, m)$. It is easy to see that H_0 is self-adjoint. Let $\tilde{V} = V(-D_\xi, \xi)$ be a pseudodifferential operator with a symbol $V \in S_{1,0}^{-\mu}(M)$ with $\mu > 1$. We suppose \tilde{V} is an H_0 -bounded self-adjoint operator on \mathcal{H} , and hence the principal symbol of \tilde{V} may be supposed to be real-valued. We write \tilde{V} and V by the same symbol for simplicity. We set

$$H = H_0 + V \quad \text{on } \mathcal{H},$$

and H is self-adjoint with $D(H) = D(H_0)$. We write

$$v(\xi) = dp_0(\xi) \in T^*M \quad \text{and} \quad M_0 = \{\xi \in M \mid v(\xi) \neq 0\}.$$

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[†]Graduate School of Mathematical Science, University of Tokyo, Tokyo, Japan, Email: shu@ms.u-tokyo.ac.jp. Partially supported by JSPS Grant Kiban (A) 21244008.

Let I be a compact interval and we assume

$$p_0^{-1}(I) = \{\xi \in M \mid p_0(\xi) \in I\} \subset M_0,$$

and $p_0^{-1}(I)$ is compact. We now consider the scattering theory for the pair (H, H_0) on the energy interval I , i.e., we study the absolutely continuous spectrum of H on I . We denote the spectral projection of an operator A on $J \subset \mathbb{R}$ by $E_J(A)$. Then the wave operators

$$W_{\pm}^I = \text{s-lim}_{t \rightarrow \pm\infty} e^{itH} e^{-itH_0} E_I(H_0)$$

exist and they are complete: $\text{Ran } W_{\pm}^I = E_I(H) \mathcal{H}_{ac}(H)$. Moreover, the point spectrum $\sigma(H) \cap I$ is finite including the multiplicities (see Section 2).

We write the energy surface of H_0 with an energy $\lambda \in I$ by

$$\Sigma_{\lambda} = p_0^{-1}(\{\lambda\}) = \{\xi \in M \mid p_0(\xi) = \lambda\}.$$

Σ_{λ} is a regular submanifold in M , and we let m_{λ} be the smooth density on Σ_{λ} characterized as follows: $m_{\lambda} = i^* \tilde{m}_{\lambda}$, where $\tilde{m}_{\lambda} \in \bigwedge^{d-1}(M)$ such that $\tilde{m}_{\lambda} \wedge dp_0 = m$, and $i : \Sigma_{\lambda} \hookrightarrow M$ is the embedding. (Note m_{λ} is uniquely determined whereas \tilde{m}_{λ} is not.) The scattering operator is defined by $S^I = (W_+^I)^* W_-^I$, $\mathcal{H} \rightarrow \mathcal{H}$, and it commutes with H_0 . Hence S^I is decomposed to a family of operators $\{S(\lambda)\}_{\lambda \in I}$, where $S(\lambda)$ is a unitary operator on $L^2(\Sigma_{\lambda}, m_{\lambda})$ for a.e. $\lambda \in I$. $S(\lambda)$ is called the scattering matrix (see Section 5 for the detail). Our main result is the following:

Theorem 1.1. *Under the above assumptions, $S(\lambda)$ is a pseudodifferential operator with its symbol in $S_{1,0}^0(\Sigma_{\lambda})$ for each $\lambda \in I \setminus \sigma_p(H)$. Moreover,*

$$\text{Sym}(S(\lambda)) = e^{-i\psi(x,\xi)} + R(x,\xi),$$

where $\text{Sym}(A)$ denotes the symbol of A ,

$$\psi(x, \xi) = \int_{-\infty}^{\infty} V(x + tv(\xi), \xi) dt \quad \text{for } \xi \in \Sigma_{\lambda}, x \in T_{\xi}^* \Sigma_{\lambda}, \quad (1.1)$$

and $R \in S_{1,0}^{-\mu}(\Sigma_{\lambda})$.

We note, in the right hand side of (1.1), we identify $T_{\xi}^* \Sigma_{\lambda}$ with a subspace of $T_{\xi}^* M$ using the Riemannian metric. We also note $\psi \in S_{1,0}^{-\mu+1}(\Sigma_{\lambda})$, and by the Taylor expansion, we have

$$e^{-i\psi(x,\xi)} = 1 - i\psi(x, \xi) + r(x, \xi), \quad r \in S_{1,0}^{-2(\mu-1)}(\Sigma_{\lambda}).$$

The first two terms in the right hand side corresponds to the classical Born approximation for the scattering matrix.

The scattering matrix is one of the central objects in the scattering theory, and a large amount of effort has been devoted to the investigation, mostly for Schrödinger operators. Chapter 8 of Yafaev's textbook [22] is an excellent reference on this subject. However, the microlocal properties of the scattering matrix seem to have attracted not much attention. One of the pioneering works is a series of papers by Isozaki and Kitada [8, 9, 10, 11], and they proved the off-diagonal smoothness of the scattering matrix using the so-called microlocal resolvent estimates. Yafaev used microlocal methods to study high energy asymptotics of the scattering matrix [21]. In these works, they have not given explicit representation of the symbol as in Theorem 1.1. For the scattering theory on scattering manifolds, Melrose and Zworski [15] showed that the scattering matrices are Fourier integral operators (see also Ito and Nakamura [13] for a generalization).

Recently, Bulger and Pushnitski have employed a sort of hybrid of the microlocal and the functional analytic methods to obtain spectral asymptotics of the scattering matrix ([4, 5]). In this paper we obtain analogous result for fixed energies using the standard pseudodifferential operator calculus on manifolds. We also mention closely related result on the spectral asymptotics by Birman and Yafaev [2], of which our result may be considered as a refinement and a generalization, if we combine our result with the Weyl formula.

One of the motivations of this work comes from applications to the scattering theory for discrete Schrödinger operators (see, e.g., Boutet de Monvel, and Sahbani [3], Isozaki and Korotyaev [12] and references therein). We can apply microlocal methods to the scattering theory of discrete Schrödinger operators by considering it as a problem on the Fourier space \mathbb{T}^d . In particular, we can show that the scattering matrix is a pseudodifferential operator on the energy surface embedded in the torus, provided the energy is non critical.

We prepare estimates on the boundary value of resolvents, usually called the limiting absorption principle, using the Mourre theory in Section 2. In Section 3, we construct Isozaki-Kitada modifiers for our model. In Section 4 we prove microlocal resolvent estimates, and combining them we prove Theorem 1.1 in Section 5. We generally follow the theory of Isozaki and Kitada [8, 9, 10, 11], but with a somewhat different point of view. We discuss applications to operators on \mathbb{R}^d in Section 6, and then applications to discrete Schrödinger operators in Section 7.

In this paper, we employ slightly nonstandard notations on pseudodifferential operator calculus. Though M is our configuration space, it is usually the Fourier variable space in applications. Thus $x \in T_\xi^*M$, $\xi \in M$, would be the space variable in the original model. In order to adjust to the standard notation in such applications, we express the cotangent bundle as

$$T^*M = \{(x, \xi) \mid \xi \in M, x \in T_\xi^*M\}.$$

Also, for a symbol $a(x, \xi)$ on T^*M , we quantize it by

$$\text{Op}(a)\varphi(\xi) = a(-D_\xi, \xi)f(\xi) = (2\pi)^{-d} \iint e^{-i(\xi-\eta)\cdot x} a(x, \eta)\varphi(\eta)d\eta dx$$

for $\varphi \in C_0^\infty(M)$ in a local coordinate system. We denote the composition of symbols a, b by $a\#b$, i.e., $\text{Op}(a\#b) = \text{Op}(a)\text{Op}(b)$. We denote the standard Hörmander symbol class on M by $S_{\rho, \delta}^m(M)$, $m \in \mathbb{R}$, $0 \leq \delta < \rho \leq 1$. Namely, $a \in S_{\rho, \delta}^m(M)$ if for any $\alpha, \beta \in \mathbb{Z}_+^d$ there is $C_{\alpha\beta} > 0$ such that

$$|\partial_x^\alpha \partial_\xi^\beta a(x, \xi)| \leq C_{\alpha\beta} \langle x \rangle^{m-\rho|\alpha|+\delta|\beta|}, \quad \text{for } \xi \in M, x \in T_\xi^*M,$$

in a local coordinate. In the following, we use only the case $\rho = 1$, $\delta = 0$.

The Fourier transform is also defined with a different signature in the exponent, i.e.,

$$\mathcal{F}^*f(x) = (2\pi)^{-d/2} \int e^{i\xi \cdot x} f(\xi) d\xi, \quad f \in C_0^\infty(\mathbb{R}^d),$$

is the Fourier transform from the \mathbb{R}_ξ^d -space to the \mathbb{R}_x^d -space, and the definition of the wave front set is also changed, namely, the directions of singularities are reversed.

We denote the Riemannian metric by $(g_{ij}(\xi))$, and length of a vector in T^*M , inner products, etc., are defined using this metric. The densities m and m_λ are not necessarily the Riemannian densities. For a pair of non-zero vectors $v, w \in \mathbb{R}^d$, we denote

$$\cos(v, w) = \frac{v \cdot w}{|v||w|} \in [-1, 1].$$

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2 Limiting absorption principle

Here we prepare basic estimates on the boundary value of resolvents using the Mourre theory [16]. These results are essentially not new (see, e.g., Amrein, Boutet de Monvel, Georgescu [1], Section 7.6), and we briefly explain the proof partly for the completeness, but also because the formulation is slightly different.

We choose $I' \ni I$ so that $p_0^{-1}(I') \subset M_0$. We also choose $\chi_1 \in C_0^\infty(M)$ such that $\text{supp} \chi_1 \subset p_0^{-1}(I')$ and $\chi_1 = 1$ on $p_0^{-1}(I)$. Then we define a vector field A_0 by

$$A_0 = \sum_{j,k=1}^d \chi_1(\xi) g^{jk}(\xi) \frac{\partial p_0}{\partial \xi_k}(\xi) \frac{\partial}{\partial \xi_j}$$

in a local coordinate. Then we set

$$A = \frac{1}{2}(iA_0 - iA_0^*) \quad \text{on } C_0^\infty(M).$$

A is essentially self-adjoint, and we denote the unique self-adjoint extension by the same symbol. Then it is easy to see

$$[H_0, iA] = \chi_1(\xi)|v(\xi)|^2$$

and that $e^{i\sigma A}H_0e^{-i\sigma A}$ and $e^{i\sigma A}Ve^{-i\sigma A}$ are H_0 -bounded operator valued C^∞ functions in $\sigma \in \mathbb{R}$. It is also easy to see that $[V, iA]$ is a compact operator under our assumptions. Thus we can apply the Mourre theory on I . Moreover, since A is relatively bounded with respect to $|D_\xi|$, we can conclude the following standard result in two-body scattering theory.

Theorem 2.1. (1) $I \cap \sigma_p(H)$ is discrete, and it is finite with their multiplicities.

(2) Let $s > 1/2$. Then for any $\lambda \in I \setminus \sigma_p(H)$,

$$(H - \lambda \mp i0)^{-1} = \lim_{\varepsilon \downarrow 0} (H - \lambda \mp i\varepsilon)^{-1}$$

exist as operators from $H^s(M)$ to $H^{-s}(M)$, and they are Hölder continuous in λ . In particular, the spectrum of H is absolutely continuous on $I \setminus \sigma_p(H)$.

(3) Let $k \in \mathbb{N}$ and let $s > k + 1/2$. Then for $\lambda \in I \setminus \sigma_p(H)$,

$$(H - \lambda \mp i0)^{-k-1} = \lim_{\varepsilon \downarrow 0} (H - \lambda \mp i\varepsilon)^{-k-1}$$

are bounded from $H^s(M)$ to $H^{-s}(M)$, and they are Hölder continuous in λ . In particular, $(H - \lambda \mp i0)^{-1}$ are C^k -class functions in $\lambda \in I \setminus \sigma_p(H)$ as operators from $H^s(M)$ to $H^{-s}(M)$.

For the abstract Mourre theory, we refer Mourre [16], Jensen, Mourre, Perry [14], Amrein, Boutet de Monvel, Georgescu [1] and Gérard [6].

3 Isozaki-Kitada modifiers

Here we construct Isozaki-Kitada type modifiers for our model. For the short range perturbation, we can construct the modifiers as pseudodifferential operators (see, Isozaki, Kitada [11]). We employ a slightly different construction from [11], which is already used, for example, in [18].

Let $I \Subset \mathbb{R}$ as before, and let

$$\Omega_\pm^\varepsilon = \{(x, \xi) \in T^*M \mid \pm \cos(x, v(\xi)) > -1 + \varepsilon, |x| > 1, p_0(\xi) \in I\}$$

with $\varepsilon > 0$. We first construct symbols a^\pm on T^*M such that, roughly speaking,

$$H\text{Op}(a^\pm) - \text{Op}(a^\pm)H_0 \sim 0 \quad \text{in } \Omega_\pm^\varepsilon,$$

and $a^\pm(x, \xi) \rightarrow 1$ as $|x| \rightarrow \infty$ in Ω_\pm^ε . We construct $a^\pm(x, \xi)$ of the form:

$$a^\pm(x, \xi) \sim e^{i\psi_\pm(x, \xi)} (1 + a_1^\pm(x, \xi) + a_2^\pm(x, \xi) + \cdots),$$

where

$$\psi_\pm(x, \xi) = \int_0^{\pm\infty} V(x + tv(\xi), \xi) dt$$

and $a_j^\pm \in S_{1,0}^{-\mu+1-j}(M)$.

We note, if $(x, \xi) \in \Omega_\pm^\varepsilon$, then $\pm \cos(x + tv(\xi), \xi) > -1 + \varepsilon$ for $\pm t \geq 0$, and

$$\begin{aligned} |x + tv(\xi)|^2 &= |x|^2 + t^2|v(\xi)|^2 + 2tx \cdot v(\xi) \\ &\geq |x|^2 + t^2|v(\xi)|^2 - 2|t|(1 - \varepsilon)|x| \cdot |v(\xi)| \\ &\geq \varepsilon(|x|^2 + |tv(\xi)|^2) \geq \frac{\varepsilon}{2}(|x| + |tv(\xi)|)^2. \end{aligned}$$

This implies, in particular, $\psi_\pm \in S_{1,0}^{-\mu+1}$ on Ω_\pm^ε . We also note ψ_\pm satisfies the transport equation:

$$v(\xi) \cdot \partial_x \psi_\pm(x, \xi) + V(x, \xi) = 0.$$

We set $a_0^\pm(x, \xi) = 1$, and we let

$$\begin{aligned} r_j^\pm(x, \xi) &= e^{-i\psi_\pm} (p_0 \# (e^{i\psi_\pm} a_j^\pm)) - (p_0 a_j^\pm - iv(\xi) \cdot \partial_x a_j^\pm + V a_j^\pm), \\ V_j^\pm(x, \xi) &= e^{-i\psi_\pm} (V \# (e^{i\psi_\pm} a_j^\pm)) - V a_j^\pm, \end{aligned}$$

for $j = 0, 1, 2, \dots$. We compute the symbol of $H\text{Op}(a^\pm) - \text{Op}(a^\pm)H_0$ formally:

$$\begin{aligned} &(p_0 + V) \# (e^{i\psi_\pm} (1 + a_1^\pm + \cdots)) - e^{i\psi_\pm} (1 + a_1^\pm + \cdots) p_0 \\ &= e^{i\psi_\pm} \left\{ \sum_{j=1}^{\infty} (-iv(\xi) \cdot \partial_x a_j^\pm(x, \xi)) + \sum_{j=0}^{\infty} r_j^\pm(x, \xi) + \sum_{j=0}^{\infty} V_j^\pm(x, \xi) \right\}. \end{aligned}$$

We solve the following equations iteratively:

$$v(\xi) \cdot \partial_x a_j^\pm(x, \xi) + ir_{j-1}^\pm(x, \xi) + iV_j^\pm(x, \xi) = 0, \quad j = 1, 2, \dots$$

We note $r_0^\pm, V_0^\pm \in S_{1,0}^{-\mu-1}$ on Ω_\pm^ε . We choose solutions as follows:

$$a_j^\pm(x, \xi) = i \int_0^{\pm\infty} (r_{j-1}^\pm(x + tv(\xi), \xi) + V_{j-1}^\pm(x + tv(\xi), \xi)) dt$$

for $j = 1, 2, \dots$, so that $a_j^\pm \in S_{1,0}^{-\mu+1-j}$ and hence $r_j^\pm, V_j^\pm \in S_{1,0}^{-\mu-1-j}$ on Ω_\pm^ε , iteratively. Then we define a^\pm as an asymptotic sum

$$a^\pm(x, \xi) \sim e^{i\psi_\pm(x, \xi)} (1 + a_1^\pm(x, \xi) + a_2^\pm(x, \xi) + \cdots), \quad (3.1)$$

which is in $S_{1,0}^0$, and $(p_0 + V)\#a^\pm - a^\pm\#p_0 \in S_{1,0}^{-\infty}$ on Ω_\pm^ε .

Now we introduce microlocal cut-off to define operators J_\pm . Let $\eta \in C^\infty([-1, 1])$ be such that

$$\eta(s) = \begin{cases} 1 & \text{if } s > -1 + \varepsilon, \\ 0 & \text{if } s < -1 + \varepsilon/2. \end{cases}$$

We fix $I_0 \Subset I$, and choose $\chi \in C_0^\infty(\mathbb{R})$ such that $\chi = 1$ on I_0 and $\text{supp}[\chi] \subset I$. Then we set

$$\tilde{a}^\pm(x, \xi) = \chi(p_0(\xi))\eta(\pm \cos(x, v(\xi)))a^\pm(x, \xi), \quad \xi \in M, x \in T_\xi^*M. \quad (3.2)$$

It is easy to see $\tilde{a}^\pm \in S_{1,0}^0(M)$, globally, and we define

$$J_\pm = \text{Op}(\tilde{a}^\pm),$$

for given $\varepsilon > 0$ and $I_0 \Subset I$. It is straightforward to verify

$$G_\pm := HJ_\pm - J_\pm H_0 = \text{Op}(g^\pm) \quad \text{with } g_\pm \in S_{1,0}^{-1}(M),$$

and

$$\begin{aligned} \text{ess-supp}[g_\pm] \subset & \{(x, \xi) \mid p_0(\xi) \in I, -1 + \varepsilon/2 \leq \pm \cos(x, v(\xi)) \leq -1 + \varepsilon\} \\ & \cup \{(x, \xi) \mid p_0(\xi) \in I \setminus I_0\}, \end{aligned} \quad (3.3)$$

where $\text{ess-supp}[a]$ denotes the essential support of a pseudodifferential operator or its symbol.

4 Microlocal resolvent estimates

Here we discuss a generalization of the microlocal resolvent estimates due to Isozaki and Kitada [8, 10]. We discuss only the two-sided microlocal resolvent estimates, which are used later. Our formulation is closer to the Hörmander type microlocal analysis than those in the papers by Isozaki and Kitada, and they are actually more precise. About closely related phase space localization estimates, we also refer a work by Mourre [17] (see also Gérard [6] for an alternative proof).

We fix $I_0 \Subset I \setminus \sigma_p(H)$, and we consider the microlocal properties of $(H - \lambda \mp i0)^{-1} : H^s(M) \rightarrow H^{-s}(M)$, $s > 1/2$, for $\lambda \in I_0$. Let $K^\pm(\lambda)$ be the distribution kernels of $(H - \lambda \mp i0)^{-1}$. For a distribution T on M , we denote the wave front set of T by $\text{WF}(T)$. When we discuss wave front sets of distributions on $M \times M$, we identify $T^*(M \times M) \cong T^*M \times T^*M$, and we denote a point in $T^*(M \times M)$ as $(x, \xi, y, \eta) \in T^*M \times T^*M$, where $\xi, \eta \in M$, $x \in T_\xi^*M$, $y \in T_\eta^*M$.

Our microlocal resolvent estimates are formulated as follows. We denote

$$\begin{aligned}\Sigma^0 &= \{(x, \xi, -x, \xi) \mid \xi \in M, x \in T_\xi^*M\}, \\ \Sigma_\pm^1(\lambda) &= \{(x + tv(\xi), \xi, -x, \xi) \mid \xi \in M, x \in T_\xi^*M, p_0(\xi) = \lambda, \pm t \geq 0\}, \\ \Sigma_\pm^2(\lambda) &= \{(tv(\xi), \xi) \mid \xi \in M, p_0(\xi) = \lambda, \pm t \geq 0\} \times T^*M, \\ \Sigma_\pm^3(\lambda) &= T^*M \times \{(tv(\xi), \xi) \mid \xi \in M, p_0(\xi) = \lambda, \pm t \geq 0\}.\end{aligned}$$

Theorem 4.1. *For $\lambda \in I \setminus \sigma_p(H)$,*

$$\text{WF}(K^\pm(\lambda)) \subset \Sigma^0 \cup \Sigma_\pm^1(\lambda) \cup \Sigma_\pm^2(\lambda) \cup \Sigma_\pm^3(\lambda).$$

Remark 4.1. Σ^0 represents the identity map on T^*M , and it comes from pseudodifferential operator type properties. As we see in Corollary 4.4, $\Sigma_\pm^1(\lambda)$ comes from the singularities of the free resolvents. $\Sigma_\pm^2(\lambda)$ and $\Sigma_\pm^3(\lambda)$ are generated by combinations of smooth off-diagonal propagations and the singularities of the free resolvents.

The microlocal resolvent estimates of Isozaki-Kitada follow easily from this:

Corollary 4.2. *Let $-1 < \mu_- < \mu_+ < 1$, and suppose $b_\pm(x, \xi) \in S_{1,0}^0(M)$ satisfy*

$$\begin{aligned}\text{ess-supp}[b_+] &\subset \{(x, \xi) \mid \cos(x, v(\xi)) \geq \mu_+, p_0(\xi) \in I_0\}, \\ \text{ess-supp}[b_-] &\subset \{(x, \xi) \mid \cos(x, v(\xi)) \leq \mu_-, p_0(\xi) \in I_0\}.\end{aligned}$$

Let $P_\pm = \text{Op}(b_\pm)$. Then $P_\mp^(H - \lambda \mp i0)^{-1}P_\pm$, $\lambda \in I_0$, are smoothing operators.*

We first consider the free resolvents, i.e., $(H_0 - \lambda \mp i0)^{-1}$.

Lemma 4.3. *For $\lambda \in I$,*

$$\text{WF}[(p_0(\xi) - \lambda \mp i0)^{-1}] = \{(tv(\xi), \xi) \mid \xi \in M, p_0(\xi) = \lambda, \pm t > 0\}.$$

Proof. This is discussed, for example, in Hörmander [7] Vol.1, Example 8.2.6. We give a proof for the sake of completeness.

It is obvious that the wave front is contained in $\{(x, \xi) \mid p_0(\xi) = \lambda\}$, and it suffices to consider the case $p_0(\xi) = \lambda$. By a partition of unity and a change of coordinates, we may assume $\lambda = 0$, $\xi = 0$ and $p_0(\xi) = \xi_1$ in a neighborhood of 0. In this case, $v(\xi) = (1, 0, \dots, 0)$.

We note

$$\mathcal{F}_1^*[(\xi \mp i0)^{-1}] = \pm\sqrt{2\pi}iF(\pm x), \quad x \in \mathbb{R},$$

where \mathcal{F}_1^* is the one-dimensional Fourier transform, and $F(x)$ is the characteristic function of $(0, \infty)$. Let $\varphi_1 \in C_0^\infty(\mathbb{R})$, $\varphi_2 \in C_0^\infty(\mathbb{R}^{d-1})$. Then by writing $\xi = (\xi_1, \xi')$, we have

$$\mathcal{F}^*[\varphi_1(\xi_1)\varphi_2(\xi')(\xi_1 \mp i0)^{-1}](x_1, x') = \pm i(\check{\varphi}_1 * F)(\pm x_1)\check{\varphi}_2(x'), \quad (x_1, x') \in \mathbb{R}^d.$$

This implies $\text{WF}[(\xi_1 \mp i0)^{-1}] = \{(t, 0, 0, \xi') \mid \pm t > 0, \xi' \in \mathbb{R}^{d-1}\}$. \square

Let $K_0^\pm(\lambda)$ be the distribution kernel of $(H_0 - \lambda \mp i0)^{-1}$. Then the above lemma implies the following characterization of the wave front set of $K_0^\pm(\lambda)$.

Corollary 4.4. *For $\lambda \in I$, $\text{WF}[K_0^\pm(\lambda)] \subset \Sigma^0 \cup \Sigma_\pm^1(\lambda)$.*

Proof. It is easy to see

$$K_0^\pm(\xi, \eta) = (p_0(\xi) - \lambda \mp i0)^{-1} \delta(\xi - \eta), \quad \xi, \eta \in M,$$

and the claim follows from a general theorem, e.g., [7] Vol.1, Proposition 8.2.10 and Lemma 4.3. One can also compute the wave front set directly, and show the equality actually holds. \square

Proof of Theorem 4.1. We fix $\lambda \in I_0 \Subset I \setminus \sigma(H)$, and we consider the “+” case only. The “−” case is proved similarly. We suppose

$$(x_1, \xi_1, -x_2, \xi_2) \notin \Sigma^0 \cup \Sigma_+^1(\lambda) \cup \Sigma_+^2(\lambda) \cup \Sigma_+^3(\lambda),$$

and we show $(x_1, \xi_1, -x_2, \xi_2) \notin \text{WF}(K^+(\lambda))$. We consider several cases separately.

Case 1: At first we consider the case $p_0(\xi_1) = p_0(\xi_2) = \lambda$. Since $x_1 \notin \{tv(\xi_1) \mid t > 0\}$ and $x_2 \notin \{tv(\xi_2) \mid t < 0\}$, we can choose $0 < \varepsilon \ll 1$ so small that

$$\cos(x_1, v(\xi_1)) < 1 - 2\varepsilon, \quad \cos(x_2, v(\xi_2)) > -1 + 2\varepsilon.$$

Then we can choose $\chi_1, \chi_2 \in S_{1,0}^0(M)$ so that they are homogeneous of order 0 in x when $|x| > 1$, $\chi_j(x_j, \xi_j) > 0$, χ_j are supported in small conic neighborhoods of (x_j, ξ_j) and hence

$$\begin{aligned} \text{supp}[\chi_1] &\subset \{(x, \xi) \mid \cos(x, v(\xi)) < 1 - \varepsilon\}, \\ \text{supp}[\chi_2] &\subset \{(x, \xi) \mid \cos(x, v(\xi)) > -1 + \varepsilon\}. \end{aligned}$$

We then construct J_\pm with this $\varepsilon > 0$ and I_0 as in the last section. By the construction, we have

$$\begin{aligned} J_+(H_0 - z)^{-1} - (H - z)^{-1} J_+ &= (H - z)^{-1} G_+(H_0 - z)^{-1}, \\ (H_0 - z)^{-1} J_-^* - J_-^*(H - z)^{-1} &= (H_0 - z)^{-1} G_-^*(H - z)^{-1} \end{aligned}$$

for $z \in \mathbb{C} \setminus \mathbb{R}$. Combining them, we obtain

$$\begin{aligned} J_-^*(H - \lambda - i0)^{-1} J_+ &= J_-^* J_+ (H_0 - \lambda - i0)^{-1} \\ &\quad - (H_0 - \lambda - i0)^{-1} J_-^* G_+(H_0 - \lambda - i0)^{-1} \\ &\quad - (H_0 - \lambda - i0)^{-1} G_-^*(H - \lambda - i0)^{-1} G_+(H_0 - \lambda - i0)^{-1}. \end{aligned} \quad (4.1)$$

By Corollary 4.4, we learn

(C-1) The wave front set of the distribution kernel of $J_-^* J_+ (H_0 - \lambda - i0)^{-1}$ is a subset of $\Sigma^0 \cup \Sigma_+^1$.

Using (3.3) and Corollary 4.4 again, we learn

(C-2) $\text{Op}(\chi_1)(H_0 - \lambda - i0)^{-1}J_-^*$ maps C^∞ functions to C^∞ functions,

(C-3) $G_+(H_0 - \lambda - i0)^{-1}\text{Op}(\chi_2)$ is smoothing,

provided χ_1 and χ_2 are supported in sufficiently small conic neighborhoods of (x_1, ξ_1) and (x_2, ξ_2) , respectively. Thus we obtain

(C-4) $\text{Op}(\chi_1)(H_0 - \lambda - i0)^{-1}J_-^*G_+(H_0 - \lambda - i0)^{-1}\text{Op}(\chi_2)$ is smoothing.

Similarly, we have

(C-5) $\text{Op}(\chi_1)(H_0 - \lambda - i0)^{-1}G_-^*$ and $G_+(H_0 - \lambda - i0)^{-1}\text{Op}(\chi_2)$ are smoothing,

(C-6) $(H - \lambda - i0)^{-1}$ is bounded from $H^s(M)$ to $H^{-s}(M)$ with $s > 1/2$ by Theorem 2.1.

Combining them, we learn

(C-7) $\text{Op}(\chi_1)(H_0 - \lambda - i0)^{-1}G_-^*(H - \lambda - i0)^{-1}G_+(H_0 - \lambda - i0)^{-1}\text{Op}(\chi_2)$ is smoothing.

From (C-4) and (C-7), we learn

(C-8) $\text{Op}(\chi_1)(J_-^*(H - \lambda - i0)^{-1}J_+ - J_-^*J_+(H_0 - \lambda - i0)^{-1})\text{Op}(\chi_2)$ is a smoothing operator, and hence its distribution kernel has no wave front set.

Noting $(x_1, \xi_1) \in \text{ess-supp}[\text{Op}(\chi_1)J_-^*]$ and $(x_2, \xi_2) \in \text{ess-supp}[J_+\text{Op}(\chi_2)]$, we conclude from (4.1), (C-1) and (C-8) that $(x_1, \xi_1, -x_2, \xi_2) \notin \text{WF}[K^+(\lambda)]$.

Case 2: We now consider the case $p_0(\xi_1) \neq \lambda$, $p_0(\xi_2) \neq \lambda$. We use the following energy localization lemma.

Lemma 4.5. *Suppose $\chi \in C_0^\infty(M)$, real-valued, and $\text{supp}[\chi] \cap \Sigma_\lambda = \emptyset$. Let $s > 1/2$. Then there is $Q \in \text{OPS}_{1,0}^0(M)$, with its symbol supported in an arbitrarily small neighborhood of $\text{supp}[\chi]$, such that*

- (1) $\chi(H - \lambda \mp i0)^{-1} - \chi Q$ is bounded from $H^s(M)$ to $C^\infty(M)$;
- (2) $(H - \lambda \mp i0)^{-1}\chi - Q\chi$ is bounded from $\mathcal{E}'(M)$ to $H^{-s}(M)$;
- (3) $\chi(H - \lambda \mp i0)^{-1}\chi - \chi Q\chi$ is smoothing, i.e., bounded from $\mathcal{E}'(M)$ to $C^\infty(M)$.

Proof. Since $H - \lambda$ is elliptic on $\text{supp}[\chi]$, one can construct a parametrix $Q \in OPS_{1,0}^0(M)$ such that

$$\chi - (H - \lambda)Q\chi = R_1$$

is smoothing. Moreover, we may assume Q is supported in an arbitrarily small neighborhood of $\text{supp}[\chi]$, and it is self-adjoint. Then we have

$$(H - \lambda \mp i0)^{-1}\chi - Q\chi = (H - \lambda \mp i0)^{-1}R_1,$$

and

$$\chi(H - \lambda \mp i0)^{-1} - \chi Q = R_1^*(H - \lambda \mp i0)^{-1}.$$

The claims (1) and (2) follow from the above expressions and the limiting absorption principle, Theorem 2.1, respectively. Combining them, we learn

$$R_2 = \chi(H - \lambda \mp i0)^{-1}\chi - \chi Q\chi$$

is bounded from $H^s(M)$ to $H^k(M)$, and also bounded from $H^{-k}(M)$ to $H^{-s}(M)$, where $s > 1/2$ and k is an arbitrary integer. By interpolation, we conclude that R_2 is bounded from $H^{-(k-s)/2}(M)$ to $H^{(k-s)/2}(M)$, and this implies R_2 is smoothing. \square

We choose $\chi \in C_0^\infty(M)$ so that $\chi(\xi_1) = \chi(\xi_2) = 1$ and $\text{supp}[\chi] \cap \Sigma_\lambda = \emptyset$. Then by Lemma 4.5 (3), we learn that $\chi(H - \lambda \mp i0)^{-1}\chi - \chi Q\chi$ is smoothing, and hence the wave front set of the distribution kernel of $\chi(H - \lambda \mp i0)^{-1}\chi$ is the same as that of $\chi Q\chi$. Since Q is a pseudodifferential operator, the wave front set of the kernel is contained in Σ^0 . Noting $\chi(\xi_1)\chi(\xi_2) = 1$ and $(x_1, \xi_1, -x_2, \xi_2) \notin \Sigma^0$, we conclude $(x_1, \xi_1, -x_2, \xi_2) \notin \text{WF}(K^+(\lambda))$.

Case 3: Suppose $p_0(\xi_1) = \lambda$ and $p_0(\xi_2) \neq \lambda$. We combine the above arguments. We choose $\varepsilon > 0$ so that $\cos(x_1, v(\xi_1)) < 1 - 2\varepsilon$, and we construct J_- as in Case 1. We also choose $\chi \in C_0^\infty(M)$ so that $\chi(\xi_2) = 1$ and $\text{supp}[\chi] \cap \Sigma_\lambda = \emptyset$ as in Case 2. We then choose $\chi_1 \in S_{1,0}^0(M)$ so that $\chi_1(x_1, \xi_1) = 1$, $\text{supp}[\chi_1] \subset \{\cos(x, v(\xi_1)) < 1 - \varepsilon\}$, and

$$\text{supp}[\chi_1] \cap \{(x, \xi) \mid \xi \in \text{supp}[\chi], x \in T_\xi^*M\} = \emptyset.$$

By Lemma 4.5, we have

$$\begin{aligned} \text{Op}(\chi_1)J_-^*(H - \lambda - i0)^{-1}\chi &= \text{Op}(\chi_1)(H_0 - \lambda - i0)^{-1}J_-^*\chi \\ &\quad - \text{Op}(\chi_1)(H_0 - \lambda - i0)^{-1}G_-^*Q\chi \\ &\quad - \text{Op}(\chi_1)(H_0 - \lambda - i0)^{-1}G_-^*(H - \lambda - i0)^{-1}R, \end{aligned}$$

where R is a smoothing operator. As in Case 1 and Case 2, we can show that each term in the right hand side is smoothing. This implies $(x_1, \xi_1, -x_2, \xi_2) \notin \text{WF}(K^+(\lambda))$.

Case 4: The case $p_0(\xi_1) \neq \lambda$ and $p_0(\xi_2) = \lambda$ is handled similarly to Case 3, and we omit the detail. \square

5 Scattering matrices

In this section we apply the results of previous sections to the scattering theory.

Proposition 5.1. *Let $I_0 \in I \setminus \sigma_p(H)$ be as in the previous sections. Then the wave operators*

$$W_{\pm}^I = \text{s-lim}_{t \rightarrow \pm\infty} e^{itH} e^{-itH_0} E_I(H_0)$$

exists and they are complete, i.e., $\text{Ran } W_{\pm}^I = E_I(H) \mathcal{H}_{ac}(H)$.

Proof. This is a standard argument, and we recall it briefly for completeness. Let $\varphi \in C_0^\infty(p_0^{-1}(I))$. Then by the non-stationary phase method, we learn that for any $N \in \mathbb{N}$,

$$\left\| \chi(-D_\xi/\varepsilon t) e^{-itH_0} \varphi \right\| \leq C_N \langle t \rangle^N, \quad t \in \mathbb{R},$$

where $\chi \in C_0^\infty(\mathbb{R}^d)$ is a smooth cut-off function such that $\chi(x) = 1$ on $\{|x| \leq 1/2\}$ and $\text{supp}[\chi] \subset \{|x| \leq 1\}$, and

$$0 < \varepsilon < \inf\{ |v(\xi)| \mid \xi \in \text{supp}[\varphi] \}.$$

The existence of the wave operators follows easily by this and the Cook-Kuroda method. The completeness follows from the limiting absorption principle, Theorem 2.1, combined with, for example, the smooth perturbation theory (see, e.g., Reed-Simon [20] Section VIII.7). \square

Then the scattering operator is defined by $S^I = (W_+^I)^* W_-^I$, and it is unitary on $E_I(H_0) \mathcal{H} = L^2(p_0^{-1}(I), m)$. Now $L^2(p_0^{-1}(I), m)$ is decomposed to

$$L^2(p_0^{-1}(I), m) \cong \int_I^\oplus L^2(\Sigma_\lambda, m_\lambda) d\lambda,$$

and the identification is given by the standard trace operator:

$$T(\lambda)\varphi(\xi) = \varphi(\xi), \quad \text{for } \xi \in \Sigma_\lambda, \varphi \in H^s(M),$$

where $s > 1/2$. Since S^I commutes with H_0 , it is decomposed to a family of operators $\{S(\lambda) \text{ on } L^2(\Sigma_\lambda, m_\lambda) \mid \lambda \in I\}$ such that

$$S(\lambda)T(\lambda)\varphi = T(\lambda)S^I\varphi \quad \text{for } \varphi \in H^s(p_0^{-1}(I)).$$

Lemma 5.2. *Let $T(\lambda)$ as above. Then*

$$T(\lambda)^* T(\lambda) = \delta(H_0 - \lambda) := \frac{1}{\pi} \text{Im} [(H_0 - \lambda - i0)^{-1}]$$

Proof. By a partition of unity and a change of coordinates, we may assume $M = \mathbb{R}^d$, $\Sigma_\lambda = \{(0, \xi') \mid \xi' \in \mathbb{R}^{d-1}\}$, and consider the operators in a small neighborhood of $0 \in \mathbb{R}^d$. We denote the velocity on Σ_λ by $dp_0(0, \xi') = (v(\xi'), 0, \dots, 0)$, the densities on M and Σ_λ by $m = m(\xi_1, \xi') d\xi_1 d\xi'$ and $m_\lambda = m_\lambda(\xi') d\xi'$, respectively. By the normalization of m_λ , we have

$$m(0, \xi') = m_\lambda(\xi') v(\xi'), \quad \xi' \in \mathbb{R}^{d-1}.$$

We now compute the operator $T(\lambda)^*$: For $\varphi \in C_0^\infty(\mathbb{R}^d)$ and $\psi \in C_0^\infty(\mathbb{R}^{d-1})$,

$$(\varphi, T(\lambda)^* \psi)_M = (T(\lambda) \varphi, \psi)_{\Sigma_\lambda} = \int_{\Sigma_\lambda} \varphi(0, \xi') \overline{\psi(\xi')} m_\lambda(\xi') d\xi'.$$

Hence, we have

$$T(\lambda)^* \psi(\xi) = \frac{m_\lambda(\xi')}{m(0, \xi')} \psi(\xi') \delta(\xi_1) = \frac{\psi(\xi')}{v(\xi')} \delta(\xi_1).$$

This implies

$$T(\lambda)^* T(\lambda) \varphi(\xi) = v(\xi')^{-1} \delta(\xi_1) \varphi(0, \xi'), \quad \varphi \in C_0^\infty(\mathbb{R}^d).$$

On the other hand, by the change of variables for distributions, we learn

$$\delta(H_0 - \lambda) = \delta(p_0(\xi) - \lambda) = v(\xi')^{-1} \delta(\xi_1)$$

and these completes the proof. \square

Let J_\pm be the Isozaki-Kitada modifiers constructed in the previous section with $0 < \varepsilon < 1$. Then the following formula is well-known.

Proposition 5.3. *For $\lambda \in I \setminus \sigma_p(H)$,*

$$S(\lambda) = -2\pi i T(\lambda) J_+^* G_- T(\lambda)^* + 2\pi i T(\lambda) G_+^* (H - \lambda - i0)^{-1} G_- T(\lambda)^*. \quad (5.1)$$

For the proof, we refer Yafaev [21], and a corresponding formula in Isozaki-Kitada [11] is essentially equivalent. The proof is functional analytic, and the computation can be carried out without any changes under our setting with the help of Lemma 5.2. In order to compute the right hand side terms, we use the following lemma.

Lemma 5.4. *Let M be a manifold with a smooth density m , and let Λ be a smooth submanifold of codimension one with a smooth density \tilde{m} . Let T be the trace operator to $\Lambda : H^s(M, m) \rightarrow L^2(\Lambda, \tilde{m})$, where $s > 1/2$. We denote the normal vector at $\xi \in \Lambda$ by $n(\xi) \in T_\xi^* M$ normalized so that $m = \hat{m} \wedge n$, where $\hat{m} \in \bigwedge^{d-1}(M)$, $i^* \hat{m} = \tilde{m}$, and $i : \Lambda \hookrightarrow M$ is the embedding.*

- (1) *Suppose $a \in S_{1,0}^{-\mu}(M)$ with $\mu > 1$. Then $T \text{Op}(a) T^*$ is a pseudo-differential operator with its symbol in $S_{1,0}^{-\mu+1}(\Lambda)$.*

(2) Suppose $a \in S_{1,0}^k(M)$, $k \in \mathbb{R}$, and suppose

$$\text{ess-supp}[a] \cap \{(\pm n(\xi), \xi) \mid \xi \in \Lambda\} = \emptyset.$$

Then $\text{TOp}(a)T^*$ is a pseudodifferential operator with its symbol in $S_{1,0}^{k+1}(\Lambda)$.

(3) Suppose either the condition of (1) or (2) is satisfied. Then the principal symbol of $\text{TOp}(a)T^*$ is given by

$$\tilde{a}(x, \xi) = \frac{1}{2\pi} \int_{-\infty}^{\infty} a(x + tn(\xi), \xi) dt, \quad \xi \in \Lambda, x \in T_{\xi}^* \Lambda. \quad (5.2)$$

Remark 5.1. We note that $x + tn(\xi)$ in (5.2) is not necessarily well-defined, since there is no canonical embedding of $T_{\xi}^* \Lambda$ into $T_{\xi}^* M$. However, the kernel of the canonical projection: $i^* : T_{\xi}^* M \rightarrow T_{\xi}^* \Lambda$ is spanned by the normal vector $n(\xi)$, and the integral in (5.2) is invariant under the translation: $(x, \xi) \mapsto (x + sn(\xi), \xi)$, $s \in \mathbb{R}$. Hence $\tilde{a}(x, \xi)$ is well-defined as a function on $T^* \Lambda$. If M is equipped with a Riemannian metric, we can naturally identify $T_{\xi}^* \Lambda$ with the normal subspace $\{n(\xi)\}^{\perp} \subset T_{\xi}^* M$, and the definition is simpler.

Proof. By a partition of unity and a change of coordinates, we may assume $M = \mathbb{R}^d$, $\Lambda = \{(0, \xi') \mid \xi' \in \mathbb{R}^{d-1}\}$, and a is supported in a small neighborhood of $0 \in \mathbb{R}^d$. We denote the normal vector by $(n(\xi'), 0, \dots, 0)$, the densities on M and Λ by $m = m(\xi_1, \xi') d\xi_1 d\xi'$ and $\tilde{m} = \tilde{m}(\xi') d\xi'$, respectively. Analogously to the proof of Lemma 5.2, we have

$$T^* \psi(\xi) = \frac{\tilde{m}(\xi')}{m(0, \xi')} \psi(\xi') \delta(\xi_1) = \frac{\psi(\xi')}{n(\xi')} \delta(\xi_1).$$

We now compute $\text{TOp}(a)T^*$ in the local coordinate:

$$\begin{aligned} \text{TOp}(a)T^* \varphi(\xi') &= (2\pi)^{-d} \iint e^{-i((0, \xi') - \eta) \cdot x} a(x_1, x', \eta_1, \eta') \frac{\varphi(\eta')}{n(\eta')} \delta(\eta_1) d\eta dx \\ &= (2\pi)^{-(d-1)} \iint e^{-i(\xi' - \eta') \cdot x'} \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} a(x_1, x', 0, \eta') \frac{dx_1}{n(\eta')} \right) \varphi(\eta') d\eta' dx' \\ &= (2\pi)^{-(d-1)} \iint e^{-i(\xi' - \eta') \cdot x'} \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} a(tn(\eta'), x', 0, \eta') dt \right) \varphi(\eta') d\eta' dx'. \end{aligned}$$

The last expression proves (5.2) for a suitable symbol $a(x, \xi)$. We can show, by direct computations, that $\tilde{a} \in S_{1,0}^{1-\mu}(\Lambda)$ if $a \in S_{1,0}^{-\mu}(M)$, $\mu > 1$. If $a \in S_{1,0}^k(M)$ satisfies the condition in (2), then in the local coordinate, we have

$$\text{ess-supp}[a] \subset \{(x_1, x', \xi_1, \xi') \mid \xi \in \Lambda, |x'| > \varepsilon |x_1|\}$$

with some $\varepsilon > 0$. Then it is straightforward to verify $\tilde{a} \in S_{1,0}^{k+1}(\Lambda)$, and we can justify the above argument. \square

Proof of Theorem 1.1. We recall the symbols of J_\pm are given by (3.2). We denote

$$Y(x, \xi) = \eta(-\cos(x, v(\xi))), \quad \xi \in M, x \in T_\xi^*M.$$

Then, by straightforward computations, we learn that the principal symbol of $J_+^*G_-$ is given by

$$\chi(p_0(\xi))^2 e^{-i\psi_+}(-i)\{p_0, Y\}e^{i\psi_-} = -ie^{-i\psi(x, \xi)}\chi(p_0(\xi))^2 v(\xi) \cdot \partial_x Y(x, \xi),$$

where

$$\psi(x, \xi) := \psi_+(x, \xi) - \psi_-(x, \xi) = \int_{-\infty}^{\infty} V(x + tv(\xi), \xi) dt.$$

It is easy to see that $\psi(x, \xi)$ is invariant under the translation: $(x, \xi) \mapsto (x + sv(\xi), \xi)$ for any $s \in \mathbb{R}$. Now we note

$$\lim_{t \rightarrow +\infty} Y(x + tv(\xi), \xi) = 0, \quad \lim_{t \rightarrow -\infty} Y(x + tv(\xi), \xi) = 1$$

for any $\xi \in p_0^{-1}(I)$ and $x \in T_\xi^*M$. We also note

$$\frac{d}{dt} Y(x + tv(\xi), \xi) = v(\xi) \cdot \partial_x Y(x + tv(\xi), \xi).$$

Combining these, we have

$$\begin{aligned} \int_{-\infty}^{\infty} v(\xi) \cdot \partial_x Y(x + tv(\xi), \xi) dt &= \lim_{T \rightarrow \infty} (Y(x + Tv(\xi), \xi) - Y(x - Tv(\xi), \xi)) \\ &= -1. \end{aligned}$$

Since $J_+^*G_-$ is essentially supported away from $\{(\pm v(\xi), \xi)\}$, we can apply Lemma 5.4 (2) to learn that $T(\lambda)J_+^*G_-T(\lambda)^*$ is a pseudodifferential operator and its principal symbol is given by

$$\frac{-i}{2\pi} \int_{-\infty}^{\infty} e^{-i\psi(x, \xi)} v(\xi) \cdot \partial_x Y(x + tv(\xi), \xi) dt = \frac{i}{2\pi} e^{-i\psi(x, \xi)}.$$

Hence the principal symbol of $-2\pi iT(\lambda)J_+^*G_-T(\lambda)^*$ is given by $e^{-i\psi(x, \xi)}$. The second term in the right hand side of (5.1) is a smoothing operator by the microlocal resolvent estimate, Corollary 4.2, and we conclude that the principal symbol of $S(\lambda)$ is given by $e^{-i\psi(x, \xi)}$ modulo the $S_{1,0}^{-1}(\Sigma_\lambda)$ terms.

In order to obtain a better remainder estimate, we use the following trick. If $V = 0$, then $S(\lambda) = 1$ for all $\lambda \in I$. This also corresponds to the case $\psi(x, \xi) = 0$ and $a^\pm(x, \xi) = 1$. Now we note

$$b^\pm(x, \xi) := \tilde{a}^\pm(x, \xi) - \chi(p_0(\xi))\eta(\pm \cos(x, v(\xi))) \in S_{1,0}^{-\mu+1}(M),$$

and we apply the above argument to $b^\pm(x, \xi)$ to conclude that the principal symbol of $S(\lambda) - I$ is given by $e^{-i\psi(x, \xi)} - 1$, and moreover, the remainder is contained in $S_{1,0}^{-\mu}(\Sigma_\lambda)$. Thus we conclude that the symbol of $S(\lambda)$ is $e^{-i\psi(x, \xi)}$ modulo the $S_{1,0}^{-\mu}(\Sigma_\lambda)$ terms. \square

6 Applications to operators on Euclidean spaces

Here we discuss applications of our main theorem to operators on Euclidean spaces, in particular Schrödinger type operators. In this section we let $M = \mathbb{R}^d$ and $\mathcal{H} = L^2(\mathbb{R}^d)$ with the standard Lebesgue measure.

Example 1. We set $p_0(\xi)$ to be a real-valued elliptic polynomial of order $2m$ on \mathbb{R}^d , and we set $H_0 = p_0(D_\xi)$ on $L^2(\mathbb{R}^d)$. We suppose $V(x, \xi)$ is a $2m$ -th order polynomial in ξ with smooth coefficients $\{a_\alpha(x)\}$, i.e.,

$$V(x, \xi) = \sum_{|\alpha| \leq 2m} a_\alpha(x) \xi^\alpha, \quad x, \xi \in \mathbb{R}^d.$$

We suppose $a_\alpha(x)$ are real-valued and there is $\mu > 1$ such that for any $\beta \in \mathbb{Z}_+^d$,

$$|\partial_x^\beta a_\alpha(x)| \leq C_\beta \langle x \rangle^{-\mu-|\beta|}, \quad x \in \mathbb{R}^d, |\alpha| \leq 2m. \quad (6.1)$$

We quantize V by

$$V = \frac{1}{2} \sum_{|\alpha| \leq 2m} (a_\alpha(x) D_x^\alpha + D_x^\alpha a_\alpha(x)),$$

then V is an infinitesimally H_0 -bounded symmetric operator. Hence $H = H_0 + V$ is a self-adjoint operator. Then we can apply Theorem 1.1 for $\hat{H} = \mathcal{F}H\mathcal{F}^*$, provided $\lambda \in \mathbb{R}$ is a non-critical value of $p_0(\xi)$. Thus the scattering matrix is a pseudodifferential operator with the principal symbol:

$$s_0(\lambda; x, \xi) = e^{-i\psi(\lambda; x, \xi)}, \quad \psi(\lambda; x, \xi) = \sum_{|\alpha| \leq 2m} \int_{-\infty}^{\infty} a_\alpha(x + tv(\xi)) \xi^\alpha dt,$$

where $p_0(\xi) = \lambda$, and $x \in \{v(\xi)\}^\perp \cong T_\xi^* \Sigma_\lambda$.

A typical example is the Schrödinger operator, i.e.,

$$H = -\frac{1}{2} \Delta + V(x),$$

where $V(x) = a_0(x)$ is supposed to satisfy the condition (6.1). In this case, $v(\xi) = \xi$ and $\Sigma_\lambda = \{\xi \in \mathbb{R}^d \mid \frac{1}{2}|\xi|^2 = \lambda\}$. Then we recover the X-ray transform type approximation ([4, 5]), i.e., the principal symbol of the scattering matrix is given by $s_0(\lambda; x, \xi) = e^{-i\psi(\lambda; x, \xi)}$, where

$$\psi(\lambda; x, \xi) = \int_{-\infty}^{\infty} V(x + t\xi) dt = \frac{1}{|\xi|} \int_{-\infty}^{\infty} V(x + t\hat{\xi}) dt$$

with $\xi \in \Sigma_\lambda$, $x \perp \xi$, $\hat{\xi} = \xi/|\xi|$. In particular, $\psi(\lambda; x, \xi)$ is homogeneous of degree $(-1/2)$ with respect to the energy $\lambda = |\xi|^2/2$.

Example 2. Another typical example is the so-called relativistic Schrödinger operator. Let $g_{ij}(x)$ be a smooth Riemannian metric on \mathbb{R}^d , $W(x)$ be a smooth real-valued function, and $m \geq 0$. We suppose there is $\mu > 1$ such that for any $\alpha \in \mathbb{Z}_+^d$,

$$|\partial_x^\alpha (g_{ij}(x) - \delta_{ij})| \leq C_\alpha \langle x \rangle^{-\mu-|\alpha|}, \quad x \in \mathbb{R}^d,$$

and

$$|\partial_x^\alpha W(x)| \leq C_\alpha \langle x \rangle^{-\mu-|\alpha|}, \quad x \in \mathbb{R}^d.$$

Then we define

$$H_0 = \sqrt{-\Delta + m^2},$$

and

$$H = \left(\sum_{i,j=1}^d D_{x_j} g_{jk}(x) D_{x_k} + m^2 \right)^{1/2} + W(x)$$

on $\mathcal{H} = L^2(\mathbb{R}^d)$. It is easy to see that H_0 and H are self-adjoint with $D(H_0) = D(H) = H^1(\mathbb{R}^d)$. Then we can show $\hat{H}_0 = \mathcal{F}H_0\mathcal{F}^{-1}$ and $\hat{H} = \mathcal{F}H\mathcal{F}^{-1}$ satisfy the assumptions of Theorem 1.1, and the result holds away from the critical value $\lambda = 0$.

We note that if $m = 0$, then the symbol of H_0 is $|\xi|$ and it has a singularity at $\xi = 0$. However, we can easily isolate the singularity using energy localization (see, e.g., Lemma 4.5). If, in addition, $g_{ij}(x) = \delta_{ij}$, then we have

$$H = |D_x| + W(x), \quad \text{and} \quad v(\xi) = \hat{\xi} = \frac{\xi}{|\xi|}.$$

By Theorem 1.1, the principal symbol of the scattering matrix is given by

$$s_0(\lambda; x, \xi) = e^{-i\psi(x, \xi)}, \quad \psi(x, \xi) = \int_{-\infty}^{\infty} W(x + t\hat{\xi}) dt,$$

where $|\xi| = \lambda$, $x \perp \xi$. We note these symbols are actually independent of the energy $\lambda > 0$.

7 Applications to discrete Schrödinger operators

In this section we discuss applications of our result to operators on the lattice \mathbb{Z}^d . We consider the Fourier space, or the dual group, \mathbb{T}^d as our configuration space, where $\mathbb{T} = \mathbb{R}/(2\pi\mathbb{Z})$.

Let \hat{H}_0 be a self-adjoint translation invariant (i.e., constant coefficients) finite difference operator on $\ell^2(\mathbb{Z}^d)$, and let $V(n)$ ($n \in \mathbb{Z}^d$) be a multiplication operator on \mathbb{Z}^d . We consider scattering theory for the pair

$$\hat{H}_0 \quad \text{and} \quad \hat{H} = \hat{H}_0 + V \quad \text{on } \ell^2(\mathbb{Z}^d).$$

We denote the discrete Fourier transform by

$$F\varphi(\xi) = (2\pi)^{-d/2} \sum_{n \in \mathbb{Z}^d} e^{-in \cdot \xi} \varphi(n), \quad \xi \in \mathbb{T}^d,$$

which is unitary from $\ell^2(\mathbb{Z}^d)$ to $L^2(\mathbb{T}^d)$. We denote the symbol of \hat{H}_0 by $p_0(\xi)$, i.e.,

$$p_0(\xi) = (2\pi)^{d/2} F(\hat{H}_0 \delta_0), \quad \text{where } \delta_0(n) = \prod_{j=1}^d \delta_{n_j, 0} \in \ell^2(\mathbb{Z}^d).$$

By the self-adjointness of \hat{H}_0 , p_0 is a real-valued trigonometric polynomial. We write

$$H_0 = F \hat{H}_0 F^* \quad \text{on } \mathcal{H} = L^2(\mathbb{T}^d),$$

and it is the multiplication operator by $p_0(\xi)$.

Now we denote the directional difference operators by

$$\tilde{\partial}_j \varphi(n) = \varphi(n) - \varphi(n - e_j), \quad n \in \mathbb{Z}^d, j = 1, \dots, d,$$

where $(e_1, \dots, e_d) \subset \mathbb{Z}^d$ is the standard basis of \mathbb{R}^d . On the potential, we suppose:

Assumption A. $V \in \ell^\infty(\mathbb{Z}^d)$, real-valued, and there is $\mu > 1$ such that for any $\alpha \in \mathbb{Z}_+^d$,

$$|\tilde{\partial}^\alpha V(n)| \leq C_\alpha \langle n \rangle^{-\mu-|\alpha|}, \quad n \in \mathbb{Z}^d,$$

with some $C_\alpha > 0$.

Under this assumption, we can show that V is extended to a real-valued smooth function \tilde{V} on \mathbb{R}^d such that for any $\alpha \in \mathbb{Z}_+^d$

$$|\partial_x^\alpha \tilde{V}(x)| \leq C_\alpha \langle x \rangle^{-\mu-|\alpha|}, \quad x \in \mathbb{R}^d,$$

with some $C_\alpha > 0$ (see, e.g., [19], Lemma 2.1). We denote the standard Fourier transform on \mathbb{R}^d by \mathcal{F} , and we let $\tilde{V}(-D_\xi) = \mathcal{F} \tilde{V}(\cdot) \mathcal{F}^*$ be a Fourier multiplier on \mathbb{R}^d .

Lemma 7.1. *We identify $\mathbb{T}^d \cong [-\pi, \pi)^d$, and let $\chi \in C_0^\infty((-\pi, \pi)^d)$. Then there is a smoothing operator K on \mathbb{T}^d such that*

$$\chi F V F^* \varphi = \chi \tilde{V}(-D_\xi) \varphi + K \varphi, \quad \varphi \in C_0^\infty((-\pi, \pi)^d).$$

Namely, $F V F^$ and $\tilde{V}(-D_\xi)$ coincide on $(-\pi, \pi)^d$ modulo the smoothing operators.*

Proof. We use an operator $\Pi : L^1(\mathbb{R}^d) \rightarrow L^1(\mathbb{T}^d)$ defined by

$$(\Pi u)(\xi) = \sum_{n \in \mathbb{Z}^d} u(\xi + 2\pi n), \quad \xi \in \mathbb{T}^d \cong [-\pi, \pi)^d, u \in L^1(\mathbb{R}^d).$$

Then we have

$$\Pi \tilde{V}(-D_\xi) \varphi(\xi) = (2\pi)^{-d} \sum_n \iint e^{-i(\xi - \eta + 2\pi n) \cdot x} \tilde{V}(x) \varphi(\eta) d\eta dx.$$

By the Poisson summation formula: $\sum_{n \in \mathbb{Z}^d} e^{2\pi i n \cdot x} = \sum_{m \in \mathbb{Z}^d} \delta(x - m)$, we learn

$$\begin{aligned} \Pi \tilde{V}(-D_\xi) \varphi(\xi) &= (2\pi)^{-d} \sum_m \iint e^{-i(\xi - \eta) \cdot x} \tilde{V}(x) \delta(x - m) \varphi(\eta) d\eta dx \\ &= (2\pi)^{-d} \sum_m \iint e^{-i(\xi - \eta) \cdot m} V(m) \varphi(\eta) d\eta \\ &= F V F^* \varphi(\xi). \end{aligned}$$

On the other hand, we write

$$\begin{aligned} \chi \tilde{V}(-D_\xi) \varphi(\xi) - \chi \Pi \tilde{V}(-D_\xi) \varphi(\xi) &= \sum_{m \neq 0} \chi(\xi) (\tilde{V}(-D_\xi) \varphi)(\xi + 2\pi m) \\ &= (2\pi)^{d/2} \int_{[-\pi, \pi)^d} \sum_{m \neq 0} \chi(\xi) (\mathcal{F} \tilde{V})(\xi - \eta + 2\pi m) \varphi(\eta) d\eta \\ &= \int_{[-\pi, \pi)^d} K(\xi, \eta) \varphi(\eta) d\eta \end{aligned}$$

with a smooth kernel $K(\xi, \eta) \in C^\infty((-\pi, \pi)^d \times (-\pi, \pi)^d)$. Thus

$$\chi F V F^* \varphi = \chi \tilde{V}(-D_\xi) \varphi - \int K(\xi, \eta) \varphi(\eta) d\eta,$$

and this completes the proof. \square

We then consider $\tilde{V}(-D_\xi)$ in the sense of pseudodifferential operator on \mathbb{T}^d . Then Lemma 7.1 implies $\tilde{V}(-D_\xi)$ and $F^* V F$ coincides modulo the smoothing operators, and thus we may consider $p(x, \xi) = p_0(\xi) + \tilde{V}(x)$ as the symbol of H . Now we can apply our results, in particular Theorem 1.1 to our model. We consider more specific examples in the rest of this section.

Example 3 (Square lattice). We consider discrete Schrödinger operators with the difference Laplacian:

$$\hat{H}_0 \varphi(n) = \frac{1}{2} \sum_{|n-m|=1} (\varphi(n) - \varphi(m)) \quad \text{for } n \in \mathbb{Z}^d, \varphi \in \ell^2(\mathbb{Z}^d),$$

and we set $\hat{H} = \hat{H}_0 + V$, where V satisfies Assumption A. Then it is easy to show

$$p_0(\xi) = \sum_{j=1}^d (1 - \cos(\xi_j)), \quad \xi \in \mathbb{T}^d,$$

and hence $\sigma(H_0) = [0, 2d]$. The velocity is given by

$$v(\xi) = (\sin(\xi_1), \dots, \sin(\xi_d)) \in \mathbb{R}^d, \quad \xi \in \mathbb{T}^d.$$

We note $v(\xi) = 0$ if and only if $\sin(\xi_j) = 0$ for $j = 1, \dots, d$. These critical points corresponds to the critical values, or the threshold energy sets, $\mathcal{T} = \{0, 2, \dots, 2d\}$.

The energy surface Σ_λ , $\lambda \in [0, 2d] \setminus \mathcal{T}$, is a regular submanifold, and it is diffeomorphic to the sphere \mathbb{S}^{d-1} , not unlike in the Euclidean space case. For $\lambda \in [0, 2d] \setminus (\mathcal{T} \cup \sigma_p(H))$, the scattering matrix $S(\lambda)$ is defined as a unitary operator on $L^2(\Sigma_\lambda, m_\lambda)$, and it is a pseudodifferential operator. Moreover, the principal symbol is given by the formula (1.1) of Theorem 1.1.

Example 4 (2D triangular lattice). Here we consider 2 dimensional triangular lattice. The configuration space is also \mathbb{Z}^2 , but the free Hamiltonian is given by

$$\hat{H}_0 \varphi(n) = \frac{1}{2} \sum_{|n-m|=1} (\varphi(n) - \varphi(m)) + \frac{1}{2} \sum_{j=\pm 1} (\varphi(n) - \varphi(n_1 + j, n_2 + j)),$$

for $\varphi \in \ell^2(\mathbb{Z}^2)$. Then the symbol is given by

$$p_0(\xi) = 3 - \cos(\xi_1) - \cos(\xi_2) - \cos(\xi_1 + \xi_2), \quad \xi = (\xi_1, \xi_2) \in \mathbb{T}^2.$$

By direct computations, we learn $v(\xi) = 0$ if and only if either (1) $\xi_1 = 0, \pi$ and $\xi_2 = 0, \pi$; or (2) $\xi_1 = \xi_2 = \pm \frac{2}{3}\pi$. Thus $p_0(\xi)$ has six critical points (one minimum, two maxima and three saddle points), and the critical values are $\mathcal{T} = \{0, 2, \frac{9}{2}\}$. The spectrum is $\sigma(H_0) = [0, \frac{9}{2}]$.

For $\lambda \in (0, 2)$, Σ_λ is diffeomorphic to the circle \mathbb{S}^1 ; for $\lambda \in (2, \frac{9}{2})$, Σ_λ has two connected components, and each is diffeomorphic to \mathbb{S}^1 . The scattering matrix $S(\lambda)$ is a pseudodifferential operator on such a manifold Σ_λ if $\lambda \in ((0, 2) \cup (2, \frac{9}{2})) \setminus \sigma_p(H)$.

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